Tsallis' entropy maximization procedure revisited

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Abstract

The proper way of averaging is an important question with regards to Tsallis' Thermostatistics. Three different procedures have been thus far employed in the pertinent literature. The third one, i.e., the Tsallis-Mendes-Plastino (TMP) [1] normalization procedure, exhibits clear advantages with respect to earlier ones. In this work, we advance a distinct (from the TMP-one) way of handling the Lagrange multipliers involved in the extremization process that leads to Tsallis' statistical operator. It is seen that the new approach considerably simplifies the pertinent analysis without losing the beautiful properties of the Tsallis-Mendes-Plastino formalism.

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I. INTRODUCTION

Tsallis' thermostatistics [1–6] is by now recognized as a new paradigm for statistical mechanical considerations. One of its crucial ingredients, Tsallis' normalized probability distribution [1], is obtained by following the well known MaxEnt route [7]. One maximizes Tsallis' generalized entropy [3,8]

$$\frac{S_q}{k} = \frac{1 - \sum_{i=1}^{w} p_i^q}{q-1}, \tag{1}$$

($k \equiv k(q)$ tends to the Boltzmann constant k_B in the limit $q \to 1$ [2]) subject to the constraints (generalized expectation values) [2]

$$\sum_{i=1}^{w} p_i = 1 \tag{2}$$

$$\frac{\sum_{i=1}^{w} p_i^q O_j^{(i)}}{\sum_{i=1}^{w} p_i^q} = \langle\langle O_j \rangle\rangle_q \,, \tag{3}$$

where p_i is the probability assigned to the microscopic configuration i ($i = 1, \ldots, w$) and one sums over all possible configurations w. $O_j^{(i)}$ ($j = 1, \ldots, n$) denote the n relevant observables (the observation level [9]), whose generalized expectation values $\langle\langle O_j \rangle\rangle_q$ are (assumedly) a priori known.

The Lagrange multipliers recipe entails maximizing [1]

$$F = \frac{S_q}{k} - \alpha_0 \left(\sum_{i=1}^{w} p_i - 1 \right) - \sum_{j=1}^{n} \lambda_j \left(\frac{\sum_{i=1}^{w} p_i^q O_j^{(i)}}{\sum_{i=1}^{w} p_i^q} - \langle\langle O_j \rangle\rangle_q \right), \tag{4}$$

yielding

$$p_i = \frac{f_i^{1/(1-q)}}{\bar{Z}_q}, \tag{5}$$

where

$$f_i = 1 - \frac{(1-q) \sum_j \lambda_j \left(O_j^{(i)} - \langle\langle O_j \rangle\rangle_q \right)}{\sum_j p_j^q}, \tag{6}$$

is the so-called configurational characteristic [10] and

$$\bar{Z}_q = \sum_i f_i^{1/(1-q)}, \tag{7}$$

stands for the partition function.

The above procedure, originally employed in [1], overcomes most of the problems posed by the old, unnormalized way of evaluating Tsallis'generalized mean values [1,11]. Some hardships remain, though. One of them is that numerical difficulties are sometimes encountered, as the p_i expression is *explicitly self-referential.* An even more serious problem is also faced: a maximum is not necessarily guaranteed. Indeed, analyzing the concomitant Hessian so as to ascertain just what kind of extreme we face, one encounters the unpleasant fact that this Hessian is not diagonal.

In the present effort we introduce an alternative Lagrange route, that overcomes the above mentioned problems.

II. THE NEW LAGRANGE MULTIPLIERS' SET

We extremize again (1) subject to the constraints (3), but, and herein lies the central idea, *rephrase* (4) by recourse to the alternative form

$$\sum_{i=1}^{w} p_i^q \left(O_j^{(i)} - \langle\langle O_j \rangle\rangle_q \right) = 0, \tag{8}$$

with $j = 1, \ldots, n$. We have now

$$F = \frac{S_q}{k} - \alpha_0 \left(\sum_{i=1}^{w} p_i - 1 \right) - \sum_{j=1}^{n} \lambda'_j \sum_{i=1}^{w} p_i^q \left(O_j^{(i)} - \langle\langle O_j \rangle\rangle_q \right), \tag{9}$$

so that, following the customary variational procedure and eliminating α_0 we find that the probabilities are, formally, still given by (5). However, in terms of the new set of Lagrange multipliers, the configurational characteristics *do not depend explicitly on the probabilities*

$$f'_i = 1 - (1-q) \sum_j \lambda'_j \left(O_j^{(i)} - \langle\langle O_j \rangle\rangle_q \right). \tag{10}$$

Comparing (10) with (6), it is clear that the Lagrange multipliers λ_j of the Tsallis-Mendes-Plastino formalism (TMP) [1] and λ'_j (present treatment) can be connected via

$$\lambda'_j = \frac{\lambda_j}{\sum_i p_i^q}, \tag{11}$$

which leads to the nice result $f_i' = f_i$. The probabilities that appear in (11) are *those special ones that maximize the entropy*, not generic ones. The ensuing, new partition function is also of the form (7), with $f_i > 0$ the well known Tsallis' cut-off condition [3,8]. Notice that now the expression for the MaxEnt probabilities p_i is NOT explicitly self-referential.

In order to ascertain the kind of extreme we are here facing we study the Hessian, that now is of *diagonal* form. The maximum condition simplifies then to the requirement

$$\frac{\partial^2 F}{\partial p_i^2} < 0. \tag{12}$$

The above derivatives are trivially performed yielding

$$\frac{\partial^2 F}{\partial p_i^2} = -q p_i^{q-2} f_i, \tag{13}$$

which formally coincides with the maximum requirement one finds in the case of Tsallis' unnormalized formalism. Since the f_i are positive-definite quantities, for a maximum one should demand that $q > 0$.

Extremes found by following the celebrated Lagrange procedure depend only on the nature of the constraints, not on the form in which they are expressed. Thus, the two sets of multipliers lead to the same numerical values for the micro-state probabilities. Via (11) one is always able to establish a connection between both treatments.

The present algorithm exhibits the same nice properties of the TMP formalism, namely:

- The MaxEnt probabilities are invariant under uniform shifts of the Hamiltonian's energy spectrum (see, for instance, the illuminating discussion of Di Sisto et al. [12]). Indeed, after performing the transformation

$$\epsilon_i \rightarrow \epsilon_i + \epsilon_0 \tag{14}$$

$$U_q \rightarrow U_q - \epsilon_0, \tag{15}$$

  on equation (5), with f_i given by (10), we trivially find that the probabilities p_i keep their forms invariant if the λ_j' do not change. Due to relation (11), the λ_j are invariant too.

- The mean value of unity equals unity, i.e., $\langle\langle 1\rangle\rangle_q = 1$, which is not the case with the unnormalized expectation values [3,8].

- One easily finds that, for two independent subsystems $A,\ B$, energies add up: $U_q(A+B) = U_q(A) + U_q(B)$.

III. OLM TREATMENT AND RÈNYI'S MEASURE

The above OLM recipe has the purpose of diagonalizing the Hessian characterizing the kind of extreme one finds after a Lagrange treatment. It is natural to ask whether the concomitant recipe works also for other information measures in addition to the Tsallis' one. We discuss next the Rènyi's measure (R_q) instance [11,13–15] in an OLM context. We have [16]

$$\frac{R_q}{k} = \frac{\ln\left[1 + (1-q)S_q\right]}{1-q}, \tag{16}$$

or (Cf. (1))

$$\frac{R_q}{k} = \frac{\ln\left(\sum_i p_i^q\right)}{q-1}. \tag{17}$$

We extremize now R_q subject to the constraints (8) with Lagrange multipiers μ_j^*. The ensuing Lagrange functional reads

$$F^* = \frac{R_q}{k} - \alpha_0\left(\sum_{i=1}^{w} p_i - 1\right) - \sum_{j=1}^{n}\mu_j^*\sum_{i=1}^{w} p_i^q\left(O_j^{(i)} - \langle\langle O_j\rangle\rangle_q\right), \tag{18}$$

whose first derivatives are

$$\frac{\partial F^*}{\partial p_i} = \frac{q p_i^{q-1}}{(q-1)\sum_i p_i^q} - \alpha_0 - q p_i^{q-1}\sum_j \mu_j^*\left(O_j^{(i)} - \langle\langle O_j\rangle\rangle_q\right) = 0. \tag{19}$$

The entropy term will lead to a self referencial probability distribution. We have

$$p_i = \frac{(f_i^*)^{\frac{1}{1-q}}}{Z_q^*}, \tag{20}$$

with a functional characteristic given by

$$f_i^* = 1 + (1-q)\sum_i p_i^q \sum_j \mu_j^* \left(O_j^{(i)} - \langle\langle O_j\rangle\rangle_q\right), \tag{21}$$

and the partition function

$$Z_q^* = \sum_i (f_i^*)^{\frac{1}{1-q}}. \tag{22}$$

We see that the OLM treatment leads to a self-referential solution that the "Rènyi-TMP" treatement does not exhibit. Indeed, on account of the fact both the constraints and the entropy share the $\sum_i p_i^q$ denominator, the TMP-Rènyi distribution has characteristics of the form [15]

$$f_i = 1 + (1-q)\sum_j \mu_j \left(O_j^{(i)} - \langle\langle O_j\rangle\rangle_q\right). \tag{23}$$

Comparing Eqs. (21) and (23), one observes that the Lagrange multipliers are connected via

$$\mu_j^* = \frac{\mu_j}{\sum_i p_i^q}, \tag{24}$$

that is the same relation found for Tsallis' measure (see Equation (11)). The following correspondence can be appreciated

$$\lambda_j' = \mu_j,$$

since the configurational characteristics of Equation (23) is identical to the one of Equation (10).

Consider now, for the second derivatives, the non-diagonal terms. One has. in the OLM instance,

$$\frac{\partial^2 F^*}{\partial p_j \partial p_i} = \frac{q^2}{1-q}\frac{(p_i p_j)^{q-1}}{\left(\sum_k p_k^q\right)^2}. \tag{25}$$

If one uses the standard TMP approach of Ref. [1] one finds, instead, for these non-diagonal terms,

$$\frac{\partial^2 F}{\partial p_j \partial p_i} = \frac{q^2}{1-q}\frac{f_i (p_i p_j)^{q-1}}{\left(\sum_k p_k^q\right)^2}. \tag{26}$$

There is an important distinction to be made between (25) and (26), that refers to the *origin* of the non-diagonal terms. In the first case, they have as a source just the entropy term of the Lagrangian. In the second, the constraints also contribute.

As a consequence we gather that the OLM approach will work as nicely as in the Tsallis case only for those measures that do not give rise to off-diagonal terms in the associated Hessian.

IV. THERMODYNAMICS

We pass now to the question of writing down the basic mathematical relationships of Thermodynamics, as expressed with respect to the new set of Lagrange multipliers λ'_j.

In order to do this in the most general quantal fashion we shall work in a basis-independent way. This requires consideration of the statistical operator (or density operator) $\hat{\rho}$ that maximizes Tsallis' entropy, subject to the foreknowledge of M generalized expectation values (corresponding to M operators $\widehat{O}_j$). These take the form

$$\left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q = \frac{Tr(\hat{\rho}^q \widehat{O}_j)}{Tr(\hat{\rho}^q)}, \qquad j = 1, ..., M. \tag{27}$$

To these we must add, of course, the normalization requirement

$$Tr\hat{\rho} = 1. \tag{28}$$

The TMP formalism, where relations are written in terms of the "old" Lagrange multipliers λ_j, yields the usual thermodynamical relationships [1], namely

$$\frac{\partial}{\partial \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q} \left(\frac{S_q}{k}\right) = \lambda_j \tag{29}$$

$$\frac{\partial}{\partial \lambda_i} (\ln_q Z_q) = - \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q , \tag{30}$$

where

$$\ln_q \bar{Z}_q = \frac{\bar{Z}_q^{1-q} - 1}{1-q} \tag{31}$$

and [1]

$$\ln_q Z_q = \ln_q \bar{Z}_q - \sum_j \lambda_j \ \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q, \tag{32}$$

so that the essential mathematical structure of Thermodynamics is preserved.

Following the standard procedure [5,16] one gets

$$\hat{\rho} = \bar{Z}_q^{-1} \left[1 - (1-q) \sum_j^M \lambda'_j \left(\widehat{O}_j - \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q \right) \right]^{\frac{1}{1-q}}, \tag{33}$$

where $\bar{Z}_q$ stands for the partition function

$$\bar{Z}_q = Tr \left[1 - (1-q) \sum_j \lambda'_j \left(\widehat{O}_j - \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q \right) \right]^{\frac{1}{1-q}}. \tag{34}$$

Enters here Tsallis'cut-off condition [5,16]. The form (33) does not a priori guarantee that we will have a positive-definite operator. Some additional considerations are requested.

Consider the operator

$$\widehat{A} \ = 1 - (1-q) \sum_j \lambda'_j \left(\widehat{O}_j - \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q \right) \tag{35}$$

enclosed within parentheses in (33). One must ensure its positive-definite character. This entails that the eigenvalues of $\hat{A}$ must be non-negative quantities. This can be achieved by recourse to an heuristic cut-off procedure. We replace (33) by

$$\hat{\rho} = \bar{Z}_q^{-1} \left[\hat{A} \ \Theta(\hat{A}) \right]^{1/(1-q)}, \tag{36}$$

with $\bar{Z}_q$ given by

$$\bar{Z}_q = Tr \left[\hat{A} \ \Theta(\hat{A}) \right]^{1/(1-q)}, \tag{37}$$

where $\Theta(x)$ is the Heaviside step-function. Equations (36)-(37) are to be re-interpreted as follows. Let $|i\rangle$ and α_i, stand, respectively, for the eigenvectors and eigenvalues of the operator (35), whose spectral decomposition is then

$$\hat{A} = \sum_i \alpha_i \ |i\rangle \langle i| \,. \tag{38}$$

In the special basis used above $\hat{\rho}$ adopts the appearance

$$\hat{\rho} = \bar{Z}_q^{-1} \sum_i f(\alpha_i) \; |i\rangle \langle i| \,, \tag{39}$$

with $f(x)$ defined as

$$f(x) = 0, \;\; for \;\; x \leq 0, \tag{40}$$

and

$$f(x) = x^{\frac{1}{1-q}}, \;\; for \;\; x > 0. \tag{41}$$

Notice that $f(x)$ possesses, for $0 < q < 1$, a continuous derivative for all x. Moreover,

$$\frac{df(x)}{dx} = \left(\frac{1}{q-1}\right) [x\Theta(x)]^{\frac{q}{1-q}} \,. \tag{42}$$

In terms of the statistical operator, Tsallis' entropy S_q reads

$$\begin{aligned} \frac{S_q}{k} &= \frac{1}{q-1} \; Tr \left[\hat{\rho}^q \left(\hat{\rho}^{1-q} - \hat{I}\right)\right] \\ &= \frac{1}{q-1} \; Tr \left[\hat{\rho}^q \left(\bar{Z}_q^{q-1} \hat{A} \; \Theta(\hat{A}) - \hat{I}\right)\right] \\ &= \frac{\bar{Z}_q^{q-1}}{q-1} \; Tr \left[\hat{\rho}^q \hat{A} \; \Theta(\hat{A})\right] - \frac{Tr(\hat{\rho}^q)}{(q-1)}, \end{aligned} \tag{43}$$

where $\hat{I}$ is the unity operator.

Obviously, $\hat{\rho}$ commutes with $\hat{A}$. The product of these two operators can be expressed in the common basis that diagonalizes them

$$\hat{\rho}^q \, \hat{A} \, \Theta(\hat{A}) = \bar{Z}_q^{-q} \sum_i [f(\alpha_i)]^q \, \alpha_i |i\rangle\langle i|, \tag{44}$$

which entails, passing from the special basis $|i\rangle$ to the general situation, that

$$\hat{\rho}^q \, \hat{A} \, \Theta(\hat{A}) = \hat{\rho}^q \left[1 - (1-q) \sum_j \lambda'_j \left(\widehat{O}_j - \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q\right)\right], \tag{45}$$

and, consequently

$$\frac{S_q}{k} = \frac{\bar{Z}_q^{q-1} - 1}{q-1} \; Tr\left(\hat{\rho}^q\right) + \bar{Z}_q^{q-1} \sum_j \lambda'_j \; Tr\left[\hat{\rho}^q \; \left(\widehat{O}_j - \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q\right)\right]. \tag{46}$$

Since the last term of the right-hand-side vanishes, by definition (8), we finally arrive at

$$\frac{S_q}{k} = \frac{\bar{Z}_q^{q-1} - 1}{q-1}\ Tr\left(\hat{\rho}^q\right). \tag{47}$$

Now, from the very definition (in terms of $\hat{\rho}$) of Tsallis' entropy S_q [5,16], we find

$$Tr\left(\hat{\rho}^q\right) = 1 + (1-q)\frac{S_q}{k}, \tag{48}$$

so that (47) and (48) lead to

$$Tr(\hat{\rho}^q) = \bar{Z}_q^{1-q} \tag{49}$$

and

$$S_q = k\ \ln_q \bar{Z}_q, \tag{50}$$

where $\ln_q \bar{Z}_q$ has been introduced in (31).

Using (49), equation (11) can be rewritten as

$$\lambda'_j = \frac{\lambda_j}{\bar{Z}_q^{1-q}}. \tag{51}$$

Following [1] we define now

$$\ln_q Z'_q = \ln_q \bar{Z}_q - \sum_j \lambda'_j\ \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q, \tag{52}$$

which leads finally to (see (29) and (30))

$$\frac{\partial}{\partial \left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q}\left(\frac{S_q}{k}\right) = \bar{Z}_q^{1-q}\lambda'_j = \lambda_j \tag{53}$$

$$\frac{\partial}{\partial \lambda'_j}\left(\ln_q Z'_q\right) = -\left\langle\left\langle \widehat{O}_j \right\rangle\right\rangle_q. \tag{54}$$

Equations (53) and (54) constitute the basic Information Theory relations on which to build up, *à la* Jaynes [7], Statistical Mechanics. Notar que OLM conduce a las mismas relaciones que TMP, y que no ha sido recesario tomar k como constante en ninguna parte del desarrollo.

As a special instance of Eqs. (53) and (54) let us discuss the Canonical Ensemble, where they adopt the appearance

$$\frac{\partial}{\partial U_q}\left(\frac{S_q}{k}\right) = \bar{Z}_q^{1-q}\beta' = \beta \tag{55}$$

$$\frac{\partial}{\partial \beta'}\left(\ln_q Z_q'\right) = -U_q, \tag{56}$$

where (see equation (52))

$$\ln_q Z_q' = \ln_q \bar{Z}_q - \beta' U_q. \tag{57}$$

Proponemos que β' Finally, the specific heat reads

$$C_q = \frac{\partial U_q}{\partial T} = \frac{\partial U_q}{\partial \beta'}\frac{d\beta'}{dT} = -\frac{\partial U_q}{\partial \beta'}\frac{1}{k'T^2} = -k'\beta'^2\frac{\partial U_q}{\partial \beta'}. \tag{58}$$

We conclude that the mathematical form of the thermodynamic relations is indeed preserved by the present treatment. Both sets of Lagrange multipliers accomplish this feat and they are connected via (11). The primed one, however, allows for a simpler treatment, as will be illustrated below.

V. SIMPLE APPLICATIONS

We consider now some illustrative examples. They are chosen in such a manner that each of them discusses a different type of situation: classical and quantal systems, the latter in the case of both finite and infinite number of levels.

A. The classical harmonic oscillator

Let us consider the classical harmonic oscillator in the canonical ensemble. We can associate with the classical oscillator a continuous energy spectrum $\epsilon(n) = \epsilon\ n$ with $\epsilon > 0$ and $n \in \mathcal{R}^+$ compatible with the cut-off condition. The ensuing MaxEnt probabilities adopt the appearance

$$p_q(n,t') = \frac{[f_q(n,t')]^{1/(1-q)}}{\bar{Z}_q(t')}, \tag{59}$$

where

$$f_q(n,t') = 1 - (1-q)\frac{(n-u_q)}{t'}, \tag{60}$$

and

$$\bar{Z}_q(t') = \int_0^{n_{max}} [f_q(n,t')]^{1/(1-q)}\, dn, \tag{61}$$

with $u_q = U_q/\epsilon$ and $t' = k'T/\epsilon$. We have introduced also n_{max} as the upper integration limit on account of Tsallis' cut-off condition. One appreciates the fact that $n_{max} \to \infty$ if $q > 1$. n_{max} is, of course, the maximum n-value that keeps $[f_q(n,t')]^{1/(1-q)} > 0$ for $q < 1$.

The normalization condition reads

$$u_q(t') = \frac{\int_0^{n_{max}} [p_q(n,t')]^q\, n\, dn}{\int_0^{n_{max}} [p_q(n,t')]^q\, dn}, \tag{62}$$

or, using (59),

$$u_q(t') = \frac{\int_0^{n_{max}} [f_q(n,t')]^{q/(1-q)}\, n\, dn}{\int_0^{n_{max}} [f_q(n,t')]^{q/(1-q)}\, dn}. \tag{63}$$

Due to the form of f_q, equation (63) constitutes a well-defined expression. By explicitly performing the integrals for $1 < q < 2$ (for $q \geq 2$ the integrals diverge) we obtain

$$u_q(t') = \frac{t'^2/(2-q)(1+(1-q)u_q/t')^{(2-q)/(1-q)}}{t'(1+(1-q)u_q/t')^{1/(1-q)}}. \tag{64}$$

After a little algebra, the above equation leads to the simple result

$$u_q(t') = t'. \tag{65}$$

Replacing now $u_q = U_q/\epsilon$ and $t' = k'T/\epsilon$, we obtain $U_q = k'T$, so that the specific heat reads

$$C_q = k'. \tag{66}$$

It is worthwhile to remark that, in the case of this particular example, we *formally* regain the usual expressions typical of the $q = 1$ case. Due to fact that we possess a degree of freedom in the definition of k', we can set $k' = k_B$ and thus recover Gibbs' Thermodynamics. Performing the pertinent integral and using (65), the partition function becomes

$$\bar{Z}_q(t') = t'(2-q)^{1/(1-q)}. \tag{67}$$

According to equation (51), t' can be written in terms of t and $\bar{Z}_q$, allowing us to recover [1]

$$\bar{Z}_q(t) = t^{1/q}(2-q)^{1/[q(1-q)]}, \tag{68}$$

and, consequently,

$$u_q = t^{1/q}(2-q)^{1/q} \tag{69}$$

$$C_q = \frac{k}{2}(2-q)^{1/q}t^{(1-q)/q}. \tag{70}$$

These results are identical to those of [1], but are here derived in a remarkably *simpler* fashion.

B. The two-level system and the quantum harmonic oscillator

Let us consider the discrete case of a single particle with an energy spectrum given by $E_n = \epsilon n$, where $\epsilon > 0$ and $n = 0, 1, ..., N$. If $N = 1$, we are facing the non degenerate two level system, while, if $n \to \infty$, the attendant problem is that of the quantum harmonic oscillator.

The micro-state probabilities are of the form, once again

$$p_n = \frac{f_n^{1/(1-q)}}{\bar{Z}_q} \tag{71}$$

with

$$\bar{Z}_q = \sum_{n=0}^{N} {f_n}^{1/(1-q)}. \tag{72}$$

The configurational characteristics take the form

$$f_n(t') = 1 - (1-q)(n-u_q)/t' \tag{73}$$

where again (see (V A)), $t' = k'T/\epsilon$ and $u_q = U_q/k'$.

Using (71), the mean energy can be written as

$$u_q = \frac{\sum_{n=0}^{N} f_n^{q/(1-q)} n}{\sum_{n=0}^{N} f_n^{q/(1-q)}}, \tag{74}$$

which, using the explicit form of f_n and rearranging terms, allows one to write down the following equation

$$\sum_{n=0}^{N} \left[1 - \frac{(1-q)}{t'}(n-u_q)\right]^{q/(1-q)} (n-u_q) = 0, \tag{75}$$

which implicitly defines u_q. Notice that one does not arrive to a closed expression. However, in order to numerically solve for u_q, we just face (75). This equation is easily solved by recourse to the so-called "seed" methods (cut-off always taken care of), with quick convergence (seconds). This is to be compared to the TMP instance [1]. In their case, one faces a non-linear coupled system of equations in order to accomplish the same task. This coupled system can be recovered from (75) and (71), writing t' in terms of t.

C. Magnetic Systems

Consider now a very simple magnetic model, discussed, for instance, in [17]: a quantum system of N spin 1/2 non-interacting atoms in the presence of a uniform, external magnetic field $\vec{H} = H\hat{k}$ (oriented along the unit vector $\hat{k}$). Each atom is endowed with a magnetic moment $\widehat{\vec{\mu}}^{(i)} = g\,\mu_0\,\widehat{\vec{S}}^{(i)}$, where $\mu_0 = e/(2mc)$ is Bohr's magneton and $\widehat{\vec{S}}^{(i)} = (\hbar/2)\,\widehat{\vec{\sigma}}^{(i)}$, with $\widehat{\vec{\sigma}}^{(i)}$ standing for the Pauli matrices. The concomitant interaction energy reads

$$\hat{\mathcal{H}} = -\sum_{i=1}^{N} \widehat{\vec{\mu}}^{(i)} \cdot \vec{H} = -\frac{g\mu_0}{\hbar} H\,\widehat{S}_z, \tag{76}$$

where $\widehat{\vec{S}} = \sum_{i=1}^{N} \widehat{\vec{S}}^{(i)}$ the total (collective) spin operator. The simultaneous eigenvectors of $\widehat{\vec{S}}^2$ and $\widehat{S}_z$ constitute a basis of the concomitant 2^N-dimensional space. We have $|S,M\rangle$, with

$S = \delta, \ldots, N/2$, $M = -S, \ldots, S$, and $\delta \equiv N/2 - [N/2] = 0$ (1/2) if N is even (odd). The corresponding multiplicities are $Y(S,M) = Y(S) = N!(2S+1)/[(N/2-S)!(N/2+S+1)!]$ [17]. We recast the Hamiltonian in the simple form

$$\hat{\mathcal{H}} = -\frac{x'}{\beta'}\hat{S}_z, \tag{77}$$

with $x' = g\mu_0 H\beta'/\hbar$. Our statistical operator can be written as

$$\hat{\rho} = \frac{1}{\bar{Z}_q}\left[1 - (1-q)x'\left(\hat{S}_z - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q\right)\right]^{1/(1-q)}, \tag{78}$$

where

$$\bar{Z}_q = Tr\left[1 - (1-q)x'\left(\hat{S}_z - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q\right)\right]^{1/(1-q)}. \tag{79}$$

Due to the cut-off condition, $1 - (1-q)x'\left(\hat{S}_z - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q\right) > 0$.

The mean value of the spin z-component is computed according to (27)

$$\left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q = \frac{Tr\left(\hat{\rho}^q \hat{S}_z\right)}{Tr\left(\hat{\rho}^q\right)}, \tag{80}$$

so that, replacing (78) into (80) and rearranging then terms we arrive at

$$Tr\left\{\left[1 + (1-q)x'\left(\hat{S}_z - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q\right)\right]^{q/(1-q)}\left(\hat{S}_z - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q\right)\right\} = 0. \tag{81}$$

More explicitly, one has

$$\sum_{S=\delta}^{N/2} Y(S) \sum_{M=-S}^{S}\left[1 + (1-q)x'\left(M - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q\right)\right]^{q/(1-q)}\left(M - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q\right) = 0, \tag{82}$$

which is the equation to be solved in order to find $\left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q$.

Notice that, once again, one faces just a *single* equation, that can be easily tackled. If one uses instead the TMP prescription (as discussed in [18]) one has to solve a *coupled*, highly non-linear system of equations. Such a system can be recovered from (82) if one replaces x' by $x/Tr(\rho^q)$ and adds the condition $Tr(\rho^q)$ from (78).

As in [18], we consider now two asymptotic situations from the present viewpoint.

For $x' \to 0$ we Taylor-expand (82) around $x' = 0$ and find

$$\left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q = \frac{qx'N}{4}, \tag{83}$$

that leads to an effective particle number

$$N^0_{eff} = qN, \tag{84}$$

as in [18]. Following the same mechanism and using (83), one finds that

$$Tr(\rho^q) = 2^{N(1-q)}. \tag{85}$$

Remembering that $x' = x/Tr(\rho^q)$, it is possible to recover the TMP normalized solution [18]

$$\left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q = \frac{qxN}{4} 2^{N(q-1)}, \tag{86}$$

and

$$N^{0\ (3)}_{eff} = qN\ 2^{N(q-1)}. \tag{87}$$

For $x' \to \infty$, and for $0 < q < 1$, expression (82) leads to an equation identical to that of [18]

$$\sum_{S=\delta}^{N/2} Y(S) \sum_{M=-S}^{S} \left(M - \left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q \right)^{1/(1-q)} = 0, \tag{88}$$

whose solution reads $\left\langle\left\langle \hat{S}_z \right\rangle\right\rangle_q = N/2$.

VI. CONCLUSIONS

In order to obtain the probability distribution p_i that maximizes Tsallis' entropy subject to appropriate constraints, Tsallis-Mendes-Plastino extremize [1]

$$F = S_q - \alpha_0 \left(\sum_{i=1}^{w} p_i - 1 \right) - \sum_{j=1}^{n} \lambda_j \left(\frac{\sum_{i=1}^{w} p_i^q O_j^{(i)}}{\sum_{i=1}^{w} p_i^q} - \langle\langle O_j \rangle\rangle_q \right),$$

and obtain

$$p_i = \frac{f_i^{1/(1-q)}}{\bar{Z}_q},$$

where

$$f_i = 1 - \frac{(1-q)\sum_j \lambda_j \left(O_j^{(i)} - \langle\langle O_j\rangle\rangle_q\right)}{k\sum_j p_j^q},$$

and $\bar{Z}_q$ is the partition function. Two rather unpleasant facts are thus faced, namely,

- p_i explicitly depends upon the probability distribution (self-reference).
- The Hessian of F is not diagonal.

In this work we have devised a transformation from the original set of Lagrange multipliers $\{\lambda_j\}$ to a new set $\{\lambda'_j\}$ such that

- Self-reference is avoided.
- The Hessian of F becomes diagonal.

As a consequence, all calculations, whether analytical or numerical, become much simpler than in [1], as illustrated with reference to several simple examples. The primed multipliers

$$\lambda'_j = \frac{\lambda_j}{\sum_i p_i^q}$$

incorporate the p_i[1] in their definition. Since one solves directly *for the primed multipliers*, such a simple step considerably simplifies the TMP treatment. Finally, we remark on the fact that the two sets of multipliers lead to thermodynamical relationships that involve identical intensive quantities (**??**).

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[1]that maximize the entropy

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